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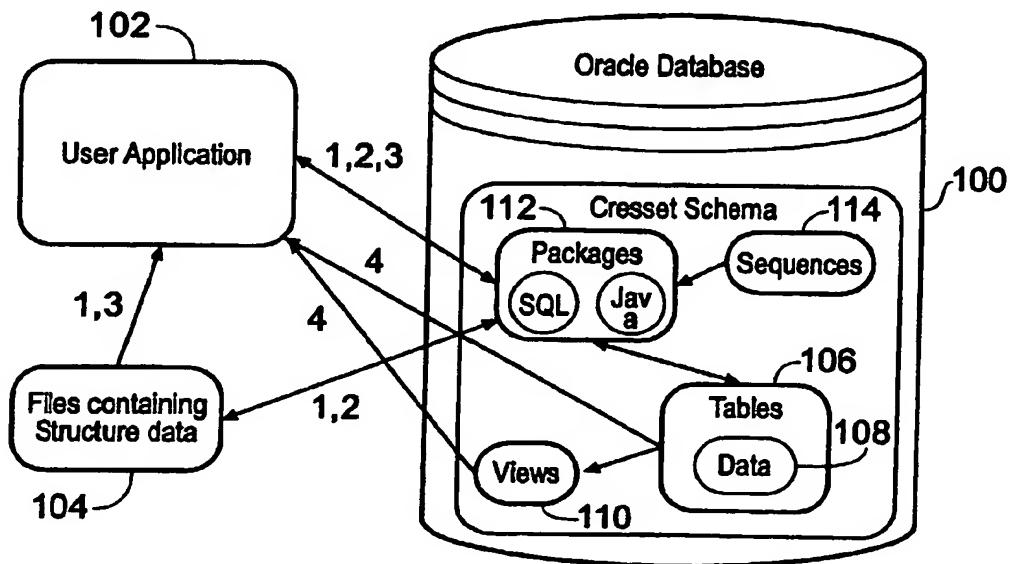
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(54) Title: SEARCHABLE MOLECULAR DATABASE



(57) Abstract: A computer system comprising a database (100) having a plurality of records is provided. Each record comprises a filed point representation representing field extrema for a conformation of a chemical structure. The database may include records for multiple conformations of the same chemical structure. Each record can have a searchable index of the filed point representation. In one embodiment the index is bit string. An indexing mechanism for generating an index, a searching mechanism for searching the database and a graphical user interface to enable a user to interface with the database (100) are also provided.



Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

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## INTERNATIONAL SEARCH REPORT

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A. CLASSIFICATION OF SUBJECT MATTER  
 IPC 7 G06F17/30 G06F17/50 G06F19/00

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, INSPEC, COMPENDEX

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	GB 2 317 030 A (XENOVA LTD) 11 March 1998 (1998-03-11)	1-7, 20, 24-31 8-19, 21-23, 32-43
Y	page 4, line 9 - line 11 page 7, line 24 - line 29 page 8, line 35 - page 9, line 15 page 11, line 6 - line 11 ---- -/-	

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	<p>XUE L GODDEN J W BAJORATH J: "Database searching for compounds with similar biological activity using short binary bit string representation of molecules"  JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES, AMERICAN CHEMICAL SOCIETY, COLUMBUS, OHIO, US,  vol. 39, no. 5, 1999, pages 881-886,  XP002958748  ISSN: 0095-2338  abstract  page 881, left-hand column, line 17  -right-hand column, line 5  page 882, left-hand column, line 1 - line 12  ----</p>	8-19, 21-23, 32-43
A	<p>FLOWER D R: "On the properties of bit string-based measures of chemical similarity"  JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES, MAY-JUNE 1998, ACS, USA,  vol. 38, no. 3, pages 379-386,  XP002267834  ISSN: 0095-2338  page 380, section "Encoding Structural Information in Bit Strings"  ----</p>	1,8,12, 16,17, 32,33, 39,40
A	<p>"XEDs : eXtended Electron Distribution"  CRESSET BIOMOLECULAR DISCOVERY LTD. WEB SITE, 'Online! 5 June 2002 (2002-06-05),  XP002267833  Retrieved from the Internet:  &lt;URL:<a href="http://web.archive.org/web/20020605204228/cresset-bmd.com/Science1.html">http://web.archive.org/web/20020605204228/cresset-bmd.com/Science1.html</a>&gt;  'retrieved on 2004-01-21!  page 1, paragraph 1  page 2, section "Validation" to page 3,  line 2  ----</p>	-/-

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>DREWRY D H ET AL: "Approaches to the design of combinatorial libraries"      CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS, ELSEVIER SCIENCE PUBLISHERS, AMSTERDAM, NL,      vol. 48, no. 1, 14 June 1999 (1999-06-14),      pages 1-20, XP004167956      ISSN: 0169-7439      page 7, left-hand column, line 24 - line 32      page 7, right-hand column, line 14 - line 25      page 9, left-hand column, line 41 - line 48      page 12, section 6.2 "Bin-based partitioning"</p> <p>---</p>	1-43
A	<p>WO 99 12113 A (MOLECULAR SIMULATIONS INC)      11 March 1999 (1999-03-11)      page 1, line 10 - line 11      page 2, line 1 - line 19      page 5, line 6 - line 12; figures 2-4      page 12, line 3 - line 24; figures 5,6</p> <p>---</p>	1,24

## INTERNATIONAL SEARCH REPORT

International Application No  
PCT/GD 3/03868

Patent document cited in search report		Publication date	Patent family member(s)		Publication date
GB 2317030	A	11-03-1998	NONE		
WO 9912113	A	11-03-1999	AT 219847 T		15-07-2002
			AU 9378098 A		22-03-1999
			CA 2302192 A1		11-03-1999
			DE 69806252 D1		01-08-2002
			EP 1010112 A1		21-06-2000
			JP 2001515249 T		18-09-2001
			WO 9912113 A1		11-03-1999
			US 6460014 B1		01-10-2002